From: Poley, David/SCO
Sent: Wednesday, June 08, 2005 12:48 PM
To: Collar, Robert/SCO
Cc: Dolegowski, John/SCO; Hartley, Jim/SAC
Subject: RE: 1,2,3-Triochloropropane Properties
Attachments: Solvent Properties.xls

Bob:

The 1,2,3-TCP solubility value of 16 mg/L, as provided in my original table, was correctly converted from Verschueren, 1983. I have not found Verschueren, 1996 yet. I have used the WHO, 2003 value of 1,750 mg/L in the updated table (attached) and, for now, will assume that the Verschueren, 1983 value is in error.

I have looked more into Henry's Law Constant (HLC) values/functions and have found that the constant is utilized in various ways - with or without units. When used without units, the dimensionless constant represents affinity of a compound for gas versus water and is expressed as a measured or empirical concentration in gas and water. The HLC is also utilized to express a chemical's volatility or solubility. Such an expression is identifiable by the units used for the HLC. Volatility expressions will have a pressure unit in the numerator, while HLC solubility expressions are inversed (will have pressure units in the denominator). See http://www.mpch-mainz.mpg.de/~sander/res/henry-conv.html for more information.

I will consider work on the attached properties table complete for now. Should you have any questions regarding the updated table, please contact me.

Thanks,

Dave

From: Collar, Robert/SCO
Sent: June 07, 2005 7:05 AM
To: Poley, David/SCO
Cc: Dolegowski, John/SCO; Hartley, Jim/SAC
Subject: FW: 1,2,3-Triochloropropane Properties

Hi Dave,

As a follow up to our conversation yesterday, I'd like to have you check some more on the properties of 1,2,3-TCP. Consequently, I am sending you the table you prepared yesterday, along with some additional information. For example, information I'd previously found on the internet suggests that the solubility for 1,2,3-TCP is 0.18 gm/100 mL which is 1.8 gm/L. Since this is close to the value of 1.75 gm/L in our draft guidance document (attached in Table A-2), I am wondering if the value of 0.016 gm/L in the table you generated yesterday is different due to some issue with units or conversion. So, I am hoping that you can look into this today.

Also, I found my old notes from grad school and it looks like the greater the Henry's Law Constant, the greater a chemical's affinity for air over water. My notes indicate that the HLC should be unitless, so I am puzzled as to why all the cited values these days have units. But, more importantly, the values in the table you generated yesterday seem to show an inverse relationship based on what I know about the four chemicals we compared: as HLC goes up, affinity for air goes down. So, I am wondering if there's some problem with units or conversions or something else. I confirmed with Ken Martins, one of our treatment engineers, that PCE should air strip the best, TCE the next best, and 1,4-dioxane the worst (poorly). This is consistent with the HLC values I've seen and my understanding of how these chemicals behave (i.e., as HLC goes up, a chemical strips better and prefers the vapor phase).

Please contact me at your convenience to discuss. Once we check on all the chemical properties and are confident of them, we can then solicit Jim Hartley's input to draft up a few sentences that describe the overall behavior of 1,2,3-TCP.

Thanks,

Bob

From: Collar, Robert/SCO
Sent: Thursday, January 20, 2005 8:35 AM
To: 'Arbaugh.Steve@epamail.epa.gov'
Cc: 'Hanusiak.Lisa@epa.gov'; ccharmley@waterboards.ca.gov; Pongetti, Paul/SCO; Ng, Melinda/LAC
Subject: 1,2,3-Triochloropropane Properties

Hi Steve,

Here's some information on the properties of 1,2,3-TCP to assist SAIC in updating their 1,2,3-TCP fact sheet. The information below is based on 1) a conversation I had with a soil gas sampling company (Environmental Support Technologies, Inc.; Curt knows of their reputation) representative, 2) data from internet web sites, and 3) internal CH2M HILL discussions and experience with 1,2,3-TCP.

1. 1,2,3-TCP should behave more like a VOC than an SVOC (semi-volatile organic compound). Attached are selected pages from the ChemFinder website (http://chemfinder.cambridgesoft.com/). These pages contain chemical property information for several chemicals that "behave" like VOCs. PCE, TCE, and 1,2,3-TCP are clearly VOCs, in particular because the methods used by labs to analyze groundwater samples for VOCs (e.g., 8260 and 524.2) have these as routine target compounds. 1,4-Dioxane is a borderline VOC/SVOC, in that it can be detected by the VOC laboratory analytical methods, but is more readily detected by SVOC laboratory analytical methods. As the term SVOC implies, 1,4-dioxane is not that volatile. And, this is one of the reasons why it is not readily amenable to soil gas surveys. However, what really affects the behavior of 1,4-dioxane and 1,2,3-TCP in the environment in the presence of water. From the attached data you'll see that 1,2,3-TCP is "insoluble" in water, with a solubility of 0.18 gm/100 mL. For comparison, TCE is less soluble in water at 0.11 gm/100 mL and PCE is even less soluble in water at 0.015 gm/100 mL. 1,4-dioxane on the other hand is "miscible" in water, which means that it "likes" to bond to water molecules, compared to sticking to itself in drops or pools in groundwater. What this all means is that 1,4-dioxane "likes" to be in groundwater and will not tend to volatilize into a vapor in the vadose zone (partially saturated region above the groundwater table) where it can be detected during soil gas sampling. At the other end of the spectrum, TCE and PCE, "aren't as happy" in groundwater and will tend to volatilize into vapor in the vadose zone, where they'll be detected during soil gas sampling. 1,2,3-TCP on the other hand falls somewhere in between the behavior of 1,4-dioxane and PCE/TCE. In other words (see below), it has a solubility that will allow it to volatilize into a vapor in the vadose zone, but not as readily as PCE or TCE. Another good web site with lots of chemical data is: http://webbook.nist.gov/chemistry/.
2. 1,2,3-TCP is amenable to detection via soil gas sampling. EST's representative said that they have analyzed for this compound during soil gas surveys, although they certainly don't target this compound for detection and analysis as often as say PCE and TCE. His recollection was that they had not detected 1,2,3-TCP during any of their surveys. There is no way of knowing why they haven't detected 1,2,3-TCP: whether it's not present, too low in concentration to be detected, or not easily detected. However, EST has detected the petroleum hydrocarbon naphthalene during soil gas surveys. This makes sense, since napthalene is less soluble in water than 1,2,3-TCP (see attached PDF file). However, another property that can influence the ability to detect a compound during soil gas surveys is the boiling point of a chemical or liquid. Water, which has a boiling point of 100 degrees centigrade, easily evaporates into a vapor. 1,2,3-TCP, with a boiling point of 156 degrees centigrade, evaporates with a bit more difficulty into a vapor, and napthalene, with a boiling point of 218 degrees centigrade requires even more heating to evaporate. So, the fact that napthalene vapors can be detected during soil gas sampling suggests that 1,2,3-TCP vapors should be detectable during soil gas sampling. For comparison, PCE and TCE, which are readily detected during soil gas sampling, have lower boiling points (closer to or less than water; see attached PDF), and vaporize relatively easily compared to 1,2,3-TCP and napthalene.
3. 1,2,3-TCP has been detected at sites around the U.S. As I mentioned previously, it's been detected in the Burbank OU in the San Fernando Valley here in southern California. The attached link shows that 1,2,3-TCP has

been detected, in particular in soil gas, at a site in New York. Understanding the behavior and detections of 1,2,3-TCP at other sites will help us to understand its fate and transport in Area 3.

4. As a contaminant migrating in groundwater, 1,2,3-TCP will behave in a manner similar to other VOCs like PCE and TCE. From the realm of groundwater treatment, 1,2,3-TCP is not readily removed by air stripping treatment. PCE and TCE are much easier to remove from groundwater via air stripping. These behaviors are consistent with 1,2,3-TCP's "desire" to dissolve more easily into water and it's tendency to be more difficult to vaporize during boiling. On the other hand, 1,2,3-TCP is readily removed from groundwater that is passed through beds of granular activated carbon for treatment. In this case, 1,2,3-TCP behaves like PCE and TCE, in that all three chemicals will have tendency to stick to carbon that might be present in a groundwater aquifer, such as in the form of organic plant matter from trees, plants, leaves, moss, etc. deposited along with sediments in lakes, rivers, and streams. What this all means is that 1,2,3-TCP migration in a groundwater aquifer will be "slowed down" or "retarded" compared to the movement of a water molecule or a chemical like chloride ion, which does not readily react with, sorb to, and be retarded by organic carbon in an aquifer.

Please let me know if you have questions about the information in this e-mail.

Thanks,

Bob

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